SOME RESULTS ON HYPERSCALING IN THE 3D ISING MODEL

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ABSTRACT

We review exact studies on finite-sized 2 dimensional Ising models and show that the point for an infinite-sized model at the critical temperature is a point of non-uniform approach in the temperature-size plane. We also illuminate some strong effects of finite-size on quantities which do not diverge at the critical point. We then review Monte Carlo studies for 3 dimensional Ising models of various sizes ($L = 2 - 100$) at various temperatures. From these results we find that the data for the renormalized coupling constant collapses nicely when plotted against the correlation length, determined in a system of edge length L, divided by L. We also find that $\xi_L/L \geq 0.26$ is definitely too large for reliable studies of the critical value, g^*, of the renormalized coupling constant. We have reasonable evidence that $\xi_L/L \approx 0.1$ is adequate for results that are within one percent of those for the infinite system size. On this basis, we have conducted a series of Monte Carlo calculations with this condition imposed. These calculations were made practical by the development of improved estimators for use in the Swendsen-Wang cluster method. We found from these results, coupled with a reversed limit computation (size increases with the temperature fixed at the critical temperature), that $g^* > 0$, although there may well be a sharp downward drop in g as the critical temperature is approached in accord with the predictions of series analysis. Our results support the validity of hyperscaling in the 3 dimensional Ising model.

We investigate the question of hyperscaling in the three dimensional Ising model by studying the renormalized coupling constant, g^*. The property of hyperscaling refers to relations between the critical indices which directly involve the spatial dimension, d. For example, just above the critical temperature, T_c,

$$\xi \propto (T - T_c)^{-\nu}, \quad C_H \propto (T - T_c)^{-\alpha}, \tag{1}$$

where ξ is the correlation length (we will be concerned here with the second moment definition) and C_H is the specific heat at constant magnetic field (H). Then a typical hyperscaling relation would be

$$d\nu = 2 - \alpha. \tag{2}$$

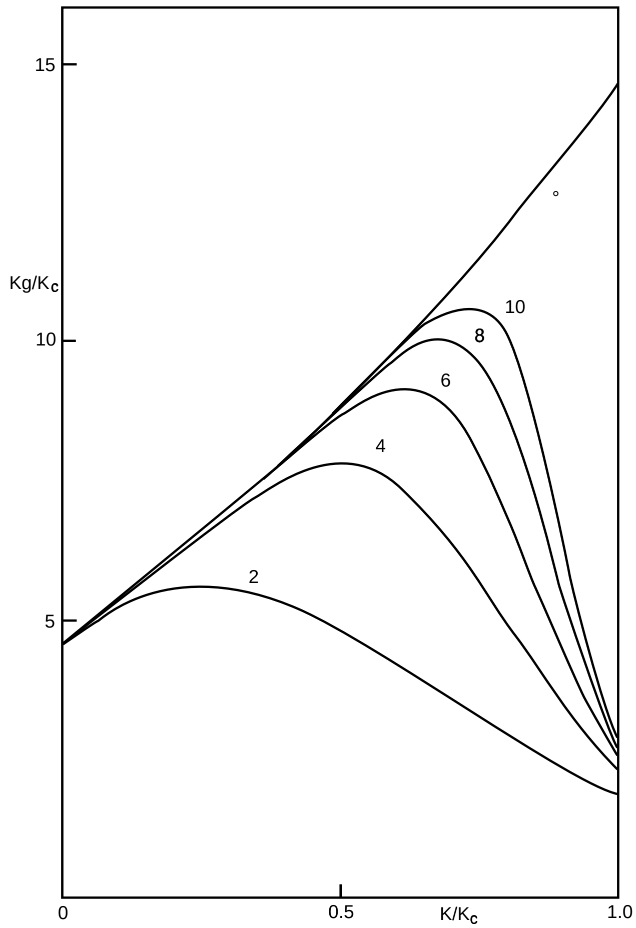

Fig. 1. Plot of gK/K_c *vs.* K. The top line is the series analysis estimate for an infinite system. The labeled curves are for $L \times L$ squares with periodic boundary conditions.

The renormalized coupling constant, has the property that if it is finite, hyperscaling holds, and hyperscaling fails if $g^* = 0$. g^* is bounded from above and can not be infinity, or negative either for that matter in the Ising model. It can be computed as the limit as the temperature approaches the critical temperature from above of

$$g(K) = -\frac{v}{a^d} \frac{\dfrac{\partial^2 \chi(K)}{\partial H^2}}{\chi^2(K)\xi^d(K)}, \tag{3}$$

$$g^* = \lim_{K \to K_c^-} \lim_{L \to \infty} g(K), \tag{4}$$

where v is the volume of a unit cell, a is the lattice spacing, $\chi(K)$ is the magnetic susceptibility, K is the exchange energy divided by the temperature, and H is the magnetic field. The limit $L \to \infty$ in (4) is to emphasis that the limit of infinite system size must be taken first. Field theoretic calculations[1] give $g(K_c, \infty) \approx 23.7$, but Tamayo and Gupta[2] give the results of their Monte Carlo calculations as $g(K_c, \text{large}) \approx 6$.

In order to better understand the nature of the problem of the computation of the renormalized coupling constant in the three dimensional Ising model, let us first consider the problem in two dimensions. We know that hyperscaling holds for this model. Baker[3] has used the Markov property method to compute the exact results for this quantity for 2, 4, 6, 8, and 10 edged square-lattices with periodic boundary conditions. His results are displayed in Fig. 1. There are several things to be observed in these results. The first is that for successively higher values of L, the finite size results agree with the infinite sized results for larger and larger values of K. The second is that at the critical temperature (which we know exactly here) the value of $g(K_c, L)$ seems stuck at low values. Baker pointed out we can compute the value of g^* when the limit is taken from the low temperature side from the results of Essam and Hunter [4]. This value is about -656, thus it is not so surprising that the value of $g(K_c, L)$ comes out to be intermediate between the thermodynamic results from the two different sides. In finite size theory this effect is thought of as "critical point rounding" because g is the ratio of divergent quantities. The other key feature for our study is, as Baker pointed out, that the finite size curves approach the limit rather more slowly than one might have anticipated. For an accuracy of about 1%, it is necessary that $\xi/L \leq 1/(7 \pm 1)$ to represent the infinite system-size limit.

The next question to be investigated therefore is the finite size behavior of the renormalized coupling constant in three dimensions. By use of a standard Monte Carlo method Baker and Erpenbech[5] have investigated this point. Their results are shown in Fig. 2. They found good data collapse when $g(K)$ was plotted against ξ_L/L, where ξ_L is the correlation length (estimated from long wave-length values of the frequency-dependent, magnetic susceptibility) found for the system of size L. It is clear from their analysis that $\xi_L/L \geq 0.26$ is definitely too large for reliable studies. They found by careful examination, include exact calculations of the results for the two-cube and the three-cube, the $\xi_L/L \approx 0.1$ seems to be sufficient for results that are within 1% of those for an infinite sized system.

With these results in mind, we have undertaken[6] a series of Monte Carlo calculations of $g(K, L)$ for the three-dimensional Ising model, being careful to use only those cases for which $\xi_L/L \approx 0.1$. This restriction poses a considerable numerical challenge because $\partial^2\chi/\partial H^2$ is the difference of two terms, each of which is about $(L/\xi)^d \approx 1000$ times larger than the answer. In order to proceed, we have developed new estimators within the framework of the Swendsen-Wang cluster algothrim. Now, in terms of the moments of the magnetization,

$$g(K, L) \equiv \left(\frac{L}{\xi}\right)^d \frac{3\langle M^2\rangle^2 - \langle M^4\rangle}{\langle M^2\rangle^2}. \tag{5}$$

It is well known that an improved estimator for the second moment of the magnetization is just the average cluster size,[7]

$$\langle M^2\rangle = \left\langle \sum_c V_c^2 \right\rangle, \tag{6}$$

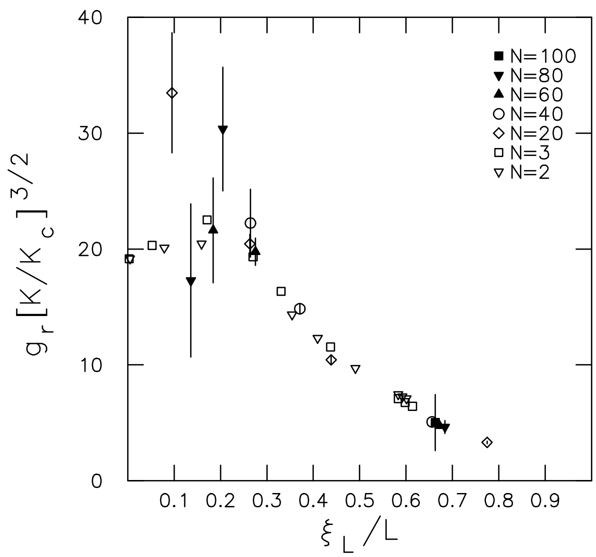

Fig. 2. Plot of $g_r(K;L)(K/K_c)^{3/2}$ for the three dimensional Ising model for the simple cubic lattice systems of size $L \times L \times L$ versus $\xi_L(K)/L$. The point for $\xi_L = 0$ is common for all values of $g(K;L)$.

where V_c is the number of sites in cluster c. For the fourth moment, we have the estimator,

$$\langle M^4 \rangle = 3 \left\langle \left(\sum_c V_c^2 \right)^2 \right\rangle - 2 \left\langle \sum_c V_c^4 \right\rangle . \tag{7}$$

For the correlation length, we follow Cooper *et al.*[8] and use,

$$f(\vec{k}) \equiv 4|\sin \vec{k}/2|^2 \left(1 - \frac{\chi(\vec{k})}{\chi} \right)^{-1}, \quad \text{with} \quad \chi(\vec{k}) \equiv \langle |M(\vec{k})|^2 \rangle / L^d, \tag{8}$$

as an estimator for ξ^{-2}, where $M(\vec{k})$ is defined by $M(\vec{k}) = \sum_{\vec{r}} \exp(-i\vec{k} \cdot \vec{r}) s_{\vec{r}}$. In the actual calcuations, we used the 6 smallest values of $|\vec{K}|$ in the determination. We have run a series of computations on this basis for cubes which are 8, 16, 32, and 64 sites on each edge, with periodic boundary conditions. The results are displayed in Fig. 3.

A few further remarks are in order here. In order to control possible systematic errors, we have computed the exact results for the 2-cube and the 3-cube at $\xi = 0.2$ and 0.3 respectively. The results for the 2-cube were 2.2% below the series estimates for an infinite system, and those for the 3-cube, 0.8% low. In addition we have run extremely long and highly accurate Monte Carlo calculations for $\xi = 0.8$ and find that they are about 0.2% below the unbiased series estimates. The series results are felt to be very accurate for these values and we believe from these comparisons that our Monte Carlo results should be within one per cent plus the Monte Carlo error of the infinite system values. The previous series results[9] which tended to zero are

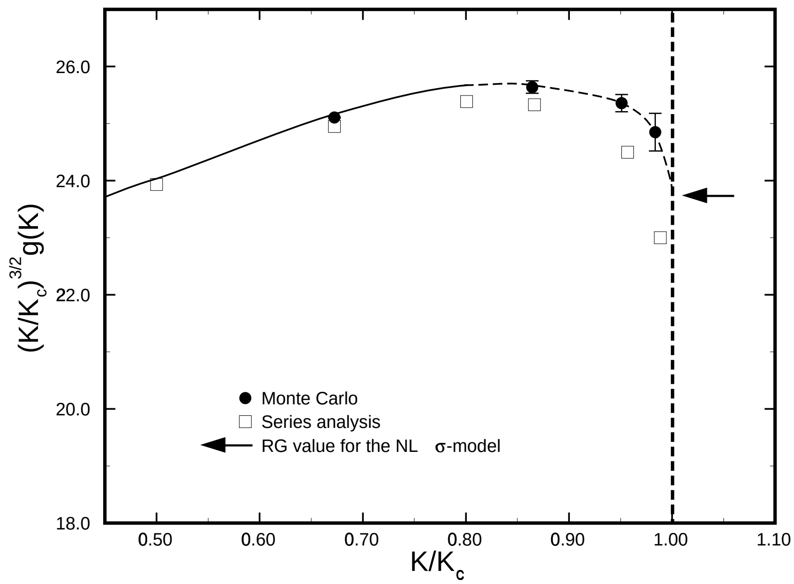

Fig. 3. The renormalized coupling constant (times $(K/K_c)^{1.5}$) *vs.* K/K_c. The solid line represents the series extrapolations as far as their apparent errors are less than the size of our dots. The dashed continuation is drawn in to guide the eye. The symbols ⫯ denote our Monte Carlo results with one-sigma error bars attached. The symbols □ are from the same type of analysis as in the work of ref. 9. Cross comparison with other analyses shows that realistic errors on this series extrapolation are sufficiently large so as not to exclude our current Monte Carlo results. The field theoretic renormalization group value is indicated by $\leftarrow$.

here seen to be too low. We believe that they did not take proper account of the subdominate terms. Our present results indicate that the value of $g* \leq 25$ and if, as indicated by the series analysis, there is a sharp drop in $g(K)$ as the critical point is approached, then our results are in reasonable accord with the field theory estimates.

We have done some further calculations beyond those which have been reported previously. We have repeated the calculations of Tamayo and Gupta[2] referred to earlier. To do this we needed an estimate of the critical temperature. Guttmann[10], using series analysis quotes $K_c = 0.221657 \pm 12$ and Ferrenberg and Landau[11] quote $K_c = 0.2216595 \pm 26$. Using the maximum spread on these two estimates to establish a temperature range for study, we have computed without attempting very high precision, the results which we show in Fig. 4. It is to be noted that to this accuracy (say plus or minus about 3% for each data point) there is no clearly discernable trend in system size over this temperature range. In two dimensions the value at K_c increases with system size. We conclude that here $g(K_c, \text{large}) \approx 5.0 \pm 0.3$, which is more or less in agreement with Tamayo and Gupta who saw a slightly larger value with larger system size. The importance of these calculations is that assuming that the structure here is the same as that of the results in two dimensions, they should provide a lower bound to g^* of about 5, which as it is greater than zero means that hyperscaling holds.

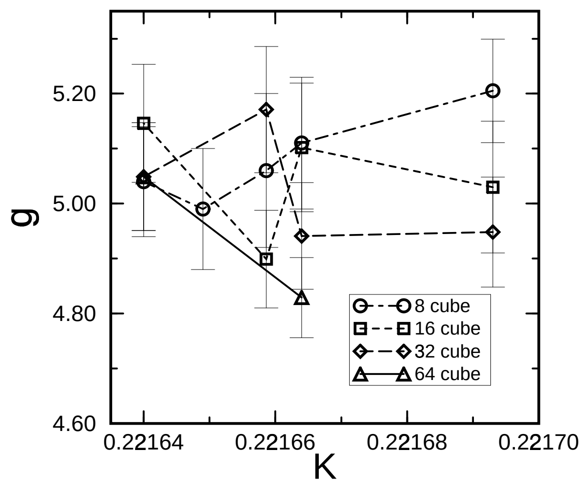

Fig. 4. The renomalized coupling constant in the neighborhood of the critical temperature for several lattice sizes.

Acknowledgements

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